MICROWAVE SPECTRUM AND IODINE NUCLEAR QUADRUPOLE COUPLING CONSTANTS OF 1,1-DIIODOETHANE

MICHAEL J. CARRILLO, WEI LIN, *Department of Chemistry, University of Texas Rio Grande Valley, Brownsville, TX, USA*; YASUKI ENDO, *Department of Applied Chemistry, National Yang Ming Chiao Tung University, Hsinchu, Taiwan*.

Only a few molecules with two iodine atoms have been studied using rotational spectroscopy probably due to the complex hyperfine splitting structure arising from the presence of two iodine nuclei. The high resolution rotational spectroscopic observation of 1,1-diiodoethane is investigated using a pulsed jet, cavity Fourier transform microwave (FTMW) spectrometer over the frequency range 11.5–18 GHz for the first time. The rotational constants, the centrifugal distortion constants, the nuclear spin-rotation coupling constants, and the complete tensor components of the nuclear quadrupole coupling for both iodine nuclei have been determined and reported. The fitted rotational constants are A = 4548.320446(47), B = 625.629141(55), C = 558.798939(43) MHz and the nuclear quadrupole coupling constants are χ_{aa} = -1089.8125(7), $\chi_{bb} - \chi_{cc}$ = -542.3162(13), $|\chi_{ab}|$ = 1215.7505(10), χ_{bc} = 340.8983(14), and $|\chi_{ac}|$ = 562.4206(19) MHz. No A-E splittings due to the methyl group internal rotation were observed. Many dipole-forbidden/electric quadrupole coupling allowed transitions were observed in the spectrum due to the large iodine quadrupole coupling effect. Quantum chemical calculations were performed at the CCSD(T)/aug-cc-pVTZ-pp level of theory. The calculated rotational constants, centrifugal distortion constants, and hyperfine constants were used to guide the data analysis.